

FILE 'REGISTRY' ENTERED AT 14:09:02 ON 06 AUG 1999
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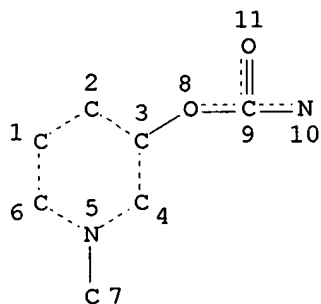
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

$\Rightarrow d$ sta que 120

Chemical structure of 1,3,5-trimethyl-2,4,6-trinitrobenzene (TNT) with atom numbering 1-15 and labels G1, O, N, Ak.

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

L17 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM

17876
SEARCH REQUEST FORMExaminer # (Mandatory): Jan Requester's Full Name: Howard ChersArt Unit 1623 Location (Bldg/Room#) En 8D12 cm1 Phone (circle 305 (306 308) 4538Serial Number: 09/029,543 Results Format Preferred (circle): PAPER DISK E-MAIL

Title of Invention _____

Inventors (please provide full names): _____

Earliest Priority Date: _____

Keywords (include any known synonyms registry numbers, explanation of initialisms):

Anion (X) = Br, I

Please see Prel. Amendment for
claims 8, 10 and 14.**Search/Topic:**

Please write detailed statement of the search topic, and the concept of the invention. Describe as specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples of relevant citations, authors, etc., if known. You may include a copy of the abstract and the broadcast or most relevant claim(s).

Please search claims 1-14.

STAFF USE ONLYSearcher: JanSearcher Phone #: 4498

Searcher Location: _____

Date Picked Up: 8/6Date Completed: 8/6Clerical Prep Time: 10Terminal Time: 15/25Number of Databases: 4**Type of Search**

____ N.A. Sequence

____ A.A. Sequence

☒ Structure (#)

____ Bibliographic

____ Litigation1

____ Fulltext

____ Procurement

____ Other

Vendors (include cost where applicable)☒ STN

____ Questel/Orbit

____ Lexis/Nexis

____ WWW/Internet

____ In-house sequence systems (list)

____ Dialog

____ Dr. Link

____ Westlaw

____ Other (specify)

t. sub

IMPORTANT INFORMATION ABOUT YOUR SEQUENCE SEARCH:

Compugen Sequence searching hardware and software explained:

This is the new sequence searching system that is currently being phased into as a replacement for the Maspar/Mpsrch platform. This system has been tested by both searchers and examiners, and has shown equivalent results to the Maspar system for the same databases. The results output format for all Compugen printed results are essentially the same except for translations.

Translation searching on Compugen explained:

The Compugen system utilizes Framesearch software for translations of proteins to nucleotides, and nucleotides to proteins. Some examiners have found these to be superior to the backtranslate software on Maspars.

FrameSearch searches a group of protein sequences for similarity to one or more nucleotide query sequences, or searches a group of nucleotide sequences for similarity to one or more protein query sequences. For each sequence comparison, the program finds an optimal alignment between the protein sequence and the corresponding codons on each the nucleotide sequence. Optimal alignments may include reading frame shifts. Please see any of the professional searching staff if you need assistance with this format.

File extensions for Compugen results transferred to floppy disks.

Compugen system search results will be delivered in one of two possible formats:

1. Standard concatenated files with .flp extension.
2. Compressed .zip files which decompressed yield two files as described below:

US08123456.cmr - Contains all commercial databases, may include Issued
US08123456.pen - Contains pending file results only

VERY IMPORTANT NOTE ABOUT PENDING FILE SEARCHES.

If your search contains file names with the following bolded extensions:

US08123456.rap US08123456.rnp

Do not leave this search in the case, during prosecution, or after the case issues, since it contains pending data which is confidential.

QUESTIONS? Contact any of the following:

Dilip Pandya, Chief, Information Branch, 308-4268

Professional searching staff:

John Dantzman (308-4488); Jan Delaval (308-4498); Mary Hale (308-4258); Barb O'Bryen (308-4291); David Schreiber (308-4292); Paula Sheppard (308-4499); Mark Spencer (308-4266); Beverly Shears (308-4994); Alex Wacławiw (308-4491).

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L19 164 SEA FILE=REGISTRY SSS FUL L17

L20 122 SEA FILE=REGISTRY SUB=L19 CSS FUL L13

100.0% PROCESSED 164 ITERATIONS

122 ANSWERS

SEARCH TIME: 00.00.01

=> d his 120-

(FILE 'REGISTRY' ENTERED AT 13:56:32 ON 06 AUG 1999)

SAV L19 HOWENS029/A

L20 122 S L13 CSS FUL SUB=L19

SAV L20 HOENS029A/A

DEL HOENS?/A

SAV L20 HOWENS029A/A

L21 102 S L20 AND (BR OR I OR CL OR F)/ELS AND NC>=2

L22 7 S L21 AND (OC5 OR OC6)/ES

L23 8 S L20 AND (OC5 OR OC6)/ES

L24 STR

L25 0 S L24 SAM SUB=L20

L26 20 S L20 NOT L21

L27 95 S L20 NOT L23,L26

L28 42 S L19 NOT L20-L23,L26,L27

L29 1 S L28 AND OC5/ES

L30 9 S L23,L29

FILE 'HCAOLD' ENTERED AT 14:08:44 ON 06 AUG 1999

L31 0 S L30

FILE 'HCAPLUS' ENTERED AT 14:08:47 ON 06 AUG 1999

L32 2 S L30

FILE 'USPATFULL' ENTERED AT 14:08:50 ON 06 AUG 1999

L33 0 S L30

FILE 'REGISTRY' ENTERED AT 14:09:02 ON 06 AUG 1999

=> d ide can tot l30

L30 ANSWER 1 OF 9 REGISTRY COPYRIGHT 1999 ACS

RN 214146-18-6 REGISTRY

CN Pyridinium, 5-[[dimethylamino)carbonyl]oxy]-2-[(.beta.-D-glucopyranosyloxy)methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

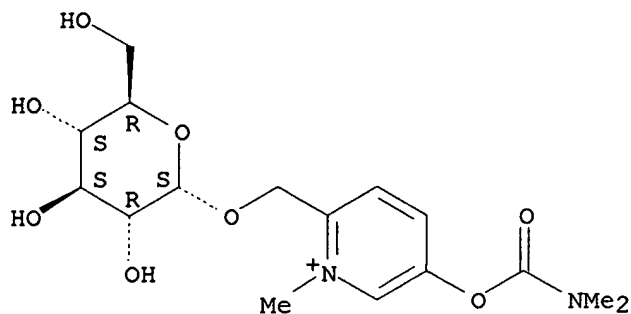
FS STEREOSEARCH

MF C16 H25 N2 O8 . Cl

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



● Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:290039

L30 ANSWER 2 OF 9 REGISTRY COPYRIGHT 1999 ACS

RN 188778-92-9 REGISTRY

CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[12-(.beta.-D-glucopyranosyloxy)dodecyl]-, bromide (9CI) (CA INDEX NAME)

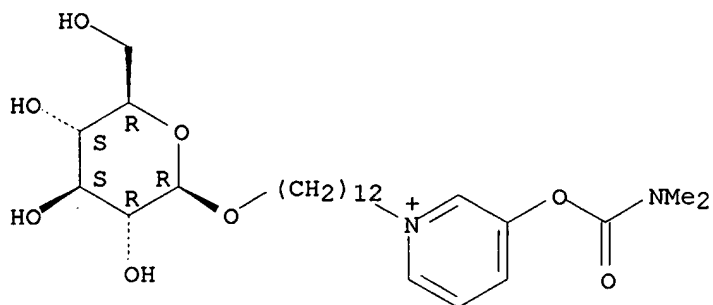
FS STEREOSEARCH

MF C26 H45 N2 O8 . Br

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



● Br⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

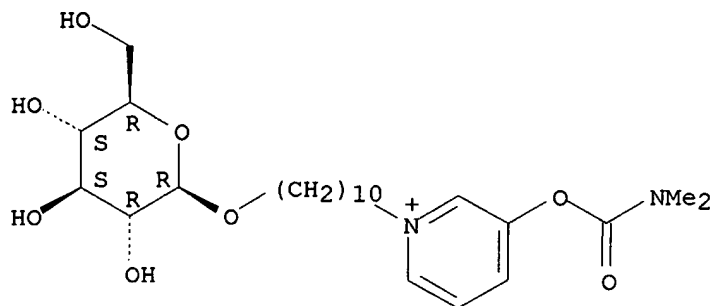
REFERENCE 1: 126:264012

L30 ANSWER 3 OF 9 REGISTRY COPYRIGHT 1999 ACS

RN 188778-91-8 REGISTRY

CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[10-(.beta.-D-glucopyranosyloxy)decyl]-, bromide (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H41 N2 O8 . Br
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



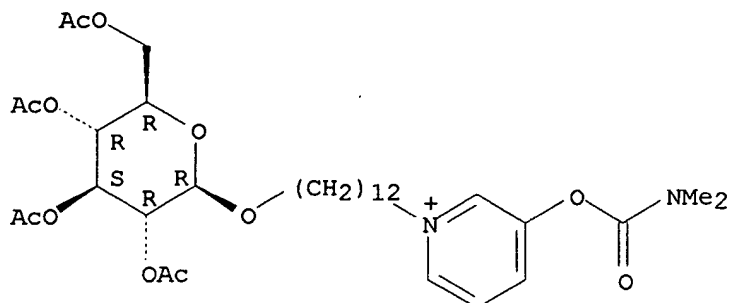
● Br⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:264012

L30 ANSWER 4 OF 9 REGISTRY COPYRIGHT 1999 ACS
RN 188778-82-7 REGISTRY
CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[12-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)oxy]dodecyl]-, bromide (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H53 N2 O12 . Br
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



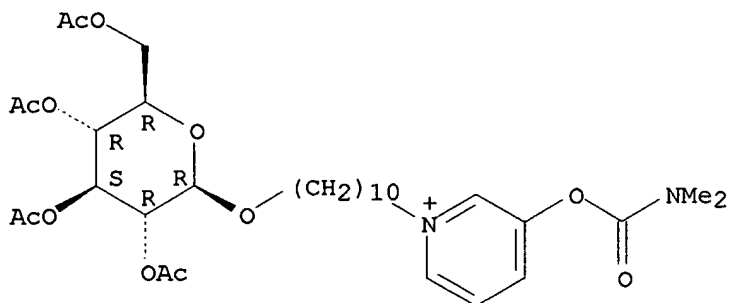
● Br⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:264012

L30 ANSWER 5 OF 9 REGISTRY COPYRIGHT 1999 ACS
RN 188778-81-6 REGISTRY
CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[10-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)oxy]decyl]-, bromide (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H49 N2 O12 . Br
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



● Br⁻

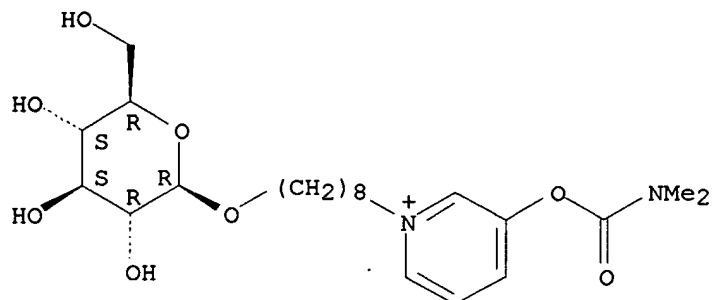
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:264012

L30 ANSWER 6 OF 9 REGISTRY COPYRIGHT 1999 ACS

RN 188778-80-5 REGISTRY
 CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[8-(.beta.-D-glucopyranosyloxy)octyl]-, chloride (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H37 N2 O8 . Cl
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



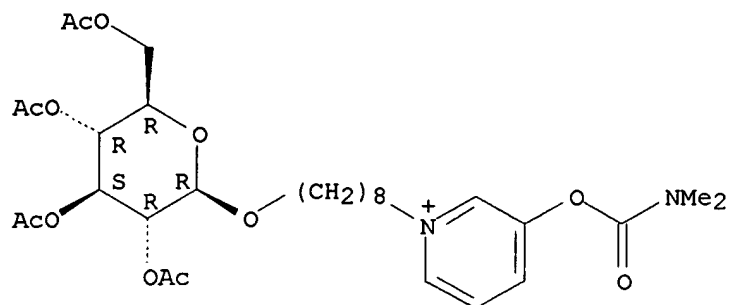
● Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:264012

L30 ANSWER 7 OF 9 REGISTRY COPYRIGHT 1999 ACS
 RN 188778-79-2 REGISTRY
 CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[8-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)oxy]octyl]-, chloride (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C30 H45 N2 O12 . Cl
 SR CA
 LC STN Files: CA, CAPLUS
 CRN (188778-77-0)

Absolute stereochemistry.



● Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

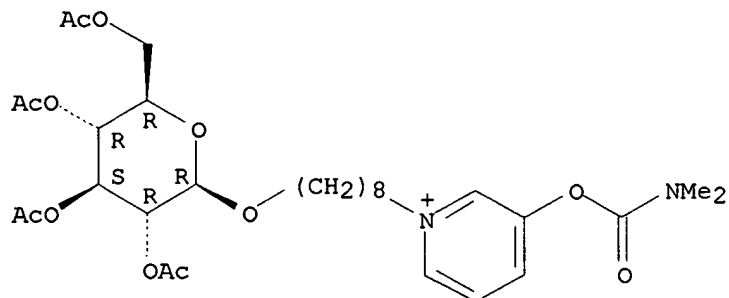
REFERENCE 1: 126:264012

L30 ANSWER 8 OF 9 REGISTRY COPYRIGHT 1999 ACS
RN 188778-78-1 REGISTRY
CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[8-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)oxy]octyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H45 N2 O12 . C F3 O3 S
SR CA
LC STN Files: CA, CAPLUS

CM 1

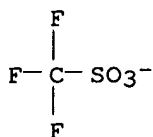
CRN 188778-77-0
CMF C30 H45 N2 O12

Absolute stereochemistry.



CM 2

CRN 37181-39-8
CMF C F3 O3 S



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:264012

L30 ANSWER 9 OF 9 REGISTRY COPYRIGHT 1999 ACS

RN 188778-77-0 REGISTRY

CN Pyridinium, 3-[[[(dimethylamino)carbonyl]oxy]-1-[8-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)oxy]octyl]- (9CI) (CA INDEX NAME)

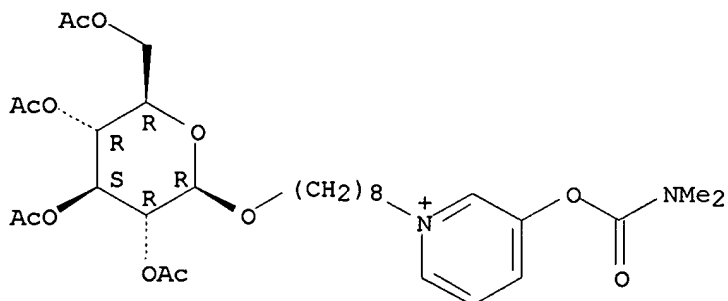
FS STEREOSEARCH

MF C30 H45 N2 O12

CI COM

SR CA

Absolute stereochemistry.



=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 14:09:23 ON 06 AUG 1999

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FILE COVERS 1967 - 6 Aug 1999 VOL 131 ISS 6

FILE LAST UPDATED: 6 Aug 1999 (19990806/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification..

This file supports REGISTRY for direct browsing and searching of

all substance data from the REGISTRY file. Enter HELP FIRST for more information.

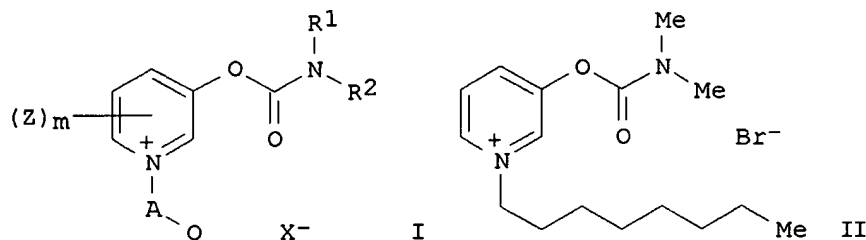
=> d 132 all tot

L32 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:565033 HCAPLUS
DN 129:290039
TI Building blocks from sugars. Part 23. Hydrophilic 3-pyridinols from fructose and isomaltulose
AU Muller, Christoph; Diehl, Volker; Lichtenthaler, Frieder W.
CS Inst. Organische Chemie, Technische Univ. Darmstadt, Darmstadt, D-64287, Germany
SO Tetrahedron (1998), 54(36), 10703-10712
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 5, 33, 63
OS CASREACT 129:290039
AB Brief exposure to bromine in water-methanol at 0.degree.C smoothly and effectively converts furfurylamine derivs. with hydroxymethyl or glucosyloxymethyl substituents into the resp. 6-substituted 3-pyridinols, whereas the N-methyl-furfurylamine derivs. elaborate the N-methyl-pyridinium betaines. Combination of this multistep one-pot reaction with the large scale-feasible generation of hydroxymethylfurfural from D-fructose and its O-glucosyl analog from isomaltulose, together with their ready conversion into furfurylamine derivs. by reductive amination, opens up a preparatively satisfactory 3-step "reaction channel" from inexpensive sugars to hydrophilic 3-pyridinols, of interest as intermediate chems. for drugs of the pyridostigmine type and agrochems.
ST hydrophilic pyridinol prepn fructose isomaltulose
IT Ring enlargement
(prepn. of hydrophilic pyridinol derivs. from fructose and isomaltulose derived hydroxymethyl- and glucosyloxymethylfurfurylamines)
IT 214146-13-1P 214146-15-3P 214146-17-5P **214146-18-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 67-47-0, 5-(Hydroxymethyl)furfural 2016-42-4, n-Tetradecylamine
88910-22-9 135100-78-6 135213-82-0
RL: RCT (Reactant)
(prepn. of hydrophilic pyridinol derivs. from fructose and isomaltulose derived hydroxymethyl- and glucosyloxymethylfurfurylamines)
IT 66357-60-6P 214146-08-4P 214146-10-8P 214146-11-9P 214146-12-0P
214146-16-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of hydrophilic pyridinol derivs. from fructose and isomaltulose derived hydroxymethyl- and glucosyloxymethylfurfurylamines)
IT 40222-77-3P, 5-Hydroxy-2-pyridinemethanol 214146-09-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of hydrophilic pyridinol derivs. from fructose and isomaltulose derived hydroxymethyl- and glucosyloxymethylfurfurylamines)

L32 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 1999 ACS
AN 1997:286379 HCAPLUS
DN 126:264012

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9708146 | A1 | 19970306 | WO 1996-IL89 | 19960829 |
| | W: AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KP, KR, LR, LT, LU, LV, MK, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, TR, UA, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | CA 2230578 | AA | 19970306 | CA 1996-2230578 | 19960829 |
| | AU 9668359 | A1 | 19970319 | AU 1996-68359 | 19960829 |
| | EP 851859 | A1 | 19980708 | EP 1996-928661 | 19960829 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE, IE, FI | | | | |
| PRAI | IL 1995-115113 | | 19950831 | | |
| | WO 1996-I | | | | |
| L89 | 19960829 | | | | |
| OS | MARPAT 126:264012 | | | | |
| GI | | | | | |



AB A series of carbamates based on the structure of pyridostigmine (PYR) were synthesized and evaluated as potential drugs for the treatment of cognitive impairments assocd. with cholinergic perturbances such as in Alzheimer's disease. The compds. are represented by structure I [R1 = H, alkyl, alkenyl, aryl, aralkyl, cycloalkyl, cycloalkylalkyl; R2 = alkyl, alkenyl, aryl aralkyl, cycloalkyl, cycloalkylalkyl; A = alk(en/yn)ylene; Z = dialkylcarbamoyl or alkyl; m = 0, 1; Q = transporter recognition moiety for biol. membranes, optionally coupled to a physiol. active acceptable moiety; X- = anion]. Compds. I were examd. for their cholinesterase inhibition, pharmacokinetics, acute toxicity, lipophilicity, reversal of scopolamine-induced memory impairment in rats (passive avoidance), and analgesia in mice. The compds. include N-alkyl-PYR derivs. and various sugar-N-alkyl-PYR conjugates, such as II. Some of the new compds. are less toxic than PYR in rats (LD50 = 5.15 mg/kg s.c.), e.g., II (LD50 = 234.8 mg/kg s.c.). Many I may serve for the treatment of other CNS-related diseases such as stroke, and PNS-related diseases such as

myasthenia gravis, glaucoma, neurogenic urinary bladder, and neuralgic pain, and as a pretreatment of organophosphorus intoxication.

ST pyridinium carbamate prepn cholinergic cognition enhancer; pyridostigmine deriv prepn acetylcholinesterase inhibitor

IT Nerve diseases
(neuralgia, treatment; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT Analgesics
Anti-Alzheimer's drugs
Antiglaucoma agents
Cholinergic agonists
Cognition enhancers
Nervous system agents
Pharmacokinetics
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT Glycosides
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT Bladder diseases
(treatment of neurogenic; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT Muscarinic antagonists
Tricyclic antidepressants
(treatment of tricyclic antidepressant side effects; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT Myasthenia gravis
Stroke
Tardive dyskinesia
(treatment; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT 9000-81-1, Acetylcholinesterase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(inhibitors; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT 188778-83-8P 188778-84-9P 188778-85-0P 188778-86-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT 155-97-5, Pyridostigmine
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT 188778-79-2P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)

IT 69440-41-1P 188778-73-6P 188778-74-7P 188778-75-8P 188778-76-9P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)

- IT 188778-78-1P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)
- IT 188778-80-5P 188778-81-6P 188778-82-7P
188778-91-8P 188778-92-9P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of pyridinium derivs. as cholinergics)
- IT 31034-86-3P, 3-Hydroxy-1-methylpyridinium bromide 68961-74-0P,
3-Hydroxy-1-decylpyridinium bromide 80635-16-1P, 3-Hydroxy-1-dodecylpyridinium bromide 188778-88-3P, 3-Hydroxy-1-butylpyridinium bromide 188778-89-4P, 3-Hydroxy-1-hexylpyridinium bromide 188778-90-7P, 3-Hydroxy-1-octylpyridinium bromide
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); MFM (Metabolic formation); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process)
(putative metabolite; prepn. and pharmacol. of pyridinium derivs. as cholinergics)
- IT 74-83-9, reactions 109-00-2, 3-Pyridinol 109-65-9, 1-Bromobutane 111-25-1, 1-Bromohexane 111-83-1, 1-Bromooctane 112-29-8, 1-Bromodecane 143-15-7, 1-Bromododecane 358-23-6, Triflic anhydride 572-09-8, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-glucopyranosyl bromide 629-41-4, 1,8-Octanediol 3344-77-2, 12-Bromo-1-dodecanol 51581-32-9, 3-(Dimethylcarbamoyloxy)pyridine 53463-68-6, 10-Bromo-1-decanol
RL: RCT (Reactant)
(starting material; prepn. and pharmacol. of pyridinium derivs. as cholinergics)